SP

OPPT-2002-0060-0023

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98 CBI? (YES/NO)

Case #:	P-99-0044	**DCN:**	
SAT Date:	10/30/98	**SAT Chair:**	V. Nabholz

RECEIVED
OPPT CBIC
98 NOV 17 AM 10:36

Submitter:

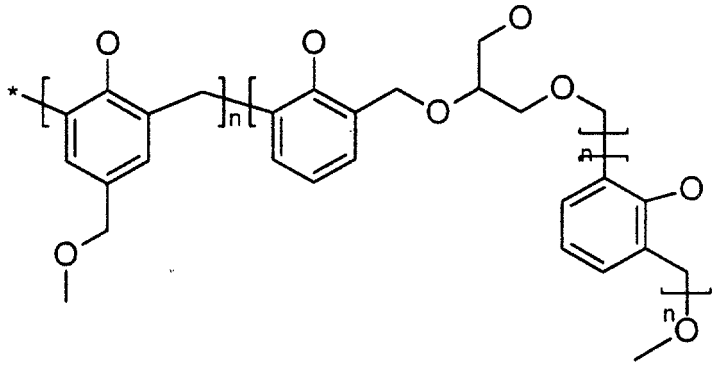
Chemical Name:

Formaldehyde, polymer with phenol and 1,2,3-propanetriol, methylated

CAS RN: 209810-57-1	**Trade Name:**

S

5099001011/1



Molecular Formula:	$C_{28}H_{33}O_8$				
Molecular Wt:	~~497~~.5704	**WT%<500:**	68.0000	**WT%<1000:**	81.0000
MP:		**BP:**		**Eq. Wt:**	
H2O Sol (g/L):	<0.001	**V.P.**		<0.000001	
Max. Prod. Volume (kg/yr):		**Physical State:**		Liquid	

USE:

Bonding agent for sand used in foundry processes. From STN/CAS on-line: no references
The PMN substance is mixed with sand and then reacted with a hardener, causing cross-linking between PMN substance and sand. This resin/sand is used to form the organic mold into which metal for castings is poured.

Related Case Numbers	Case Role	Related Case Numbers	Case Role

Focus Date: NOV 9 1998 **Results:** 5E CATEGORY Ecotox / Exposure based Eco + Fate

STRUCTURE ACTIVITY TEAM REPORT 30 October 1998 CBI

CASE NUMBER: ~~P~~99-0044

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN:	HEALTH	ECOTOX
LEVEL:	1-2	3

KEYWORDS: AQUATOX (A,C), DEVEL, SENS-S, IRR, BLOOD

SUMMARY OF ASSESSMENT:

FATE: with 81% <1000 and 68% <500;
liquid,
log K_{ow} = 2.4 (SRC);
S < 1.0 mg/L @ 20 °C (ICB), <600 mg/L (EAB);
vp < 1.0E-6 mm Hg or torr @ 25 °C;
bp >400 °C (P);
H < 1.0E-8;
log K_{oc} = 1.4 (P);
log fish BCF = 0.49 (P);
POTW removal = 0%;
time for complete ultimate aerobic biodegradation = months;
sorption to soils and sediments = low;
indirect photolysis will be rapid;
PBT Potential: P2B1T2
*CEB FATE: migration to ground water = rapid;

HEALTH: Absorption moderate all routes based on analogs;

concern for developmental toxicity, sensitization, irritation to membranes, and blood toxicity from the LMW phenols;

low to moderate concern.
*CEB HEALTH: Exposures to humans: inhalation, dermal, ingestion, and drinking water; XB: Testing desired.

ECOTOX: Predicted (P) and measured (M) toxicity values in mg/L (ppm) are:

fish 96-h LC50	=	0.160 P
daphnid 48-h LC50	=	0.150 P
green algal 96-h EC50	=	0.820 P
fish 30-d ChV	=	0.020 P
fish 90-d ChV	<	0.020 P
daphnid ChV	=	0.020 P
algal ChV	=	0.390 P

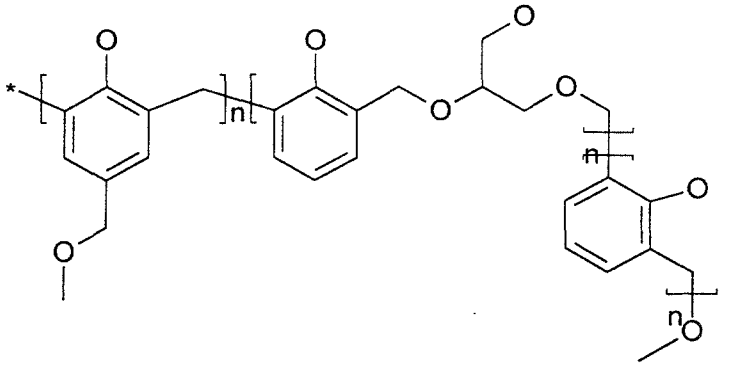
Predictions are based on SAR-nearest analog method for polyphenols; SAR chemical class = phenols-poly; with 81% <1000 and 68% <500; pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; hardness <180.0 mg/L

as CaCO3; and TOC <2.0 mg/L;
high concern;
assessment factor = 10.0
concern concentration = 0.002
*CEB ECOTOX: All releases to water; XB: Testing desired.

SAT Co-chairperson: Vince Nabholz, 260-1271

NCSAB SAT REPORT		CBI? (Y/N):
PMN:	P-99-0044	CAS RN: 209810-57-1
Chemical Name: Formaldehyde, polymer with phenol and 1,2,3-propanetriol, methylated		Analogs:
		Production Volume:

Structure:



Use:
Bonding agent for sand used in foundry processes.
From STN/CAS on-line: no references
The PMN substance is mixed with sand and then reacted with a hardener, causing cross-linking between PMN substance and sand. This resin/sand is used to form the organic mold into which metal for castings is poured.

Formula:	$C_{28}H_{33}O_8$		Eq Wt:			
Mol Weight:	~~497.57~~	Wt%<500:	68.00	Wt%<1000	81.00	
MP:		BP:		VP:	<0.000001	
H2O Sol (g/L):	<1.0	<0.001	Physical State:	Liquid	Log P:	

Endpoint (mg/L)	Est. Value	Meas. Value	Comments
Fish 96-h	0.16		worst-case analogue
Daphnid 48-h	0.15		
Algal 96-h	0.82		
Fish ChV	0.016		
Daphnid ChV	0.015		
Algal ChV	0.39		
BCF			

CHEMICAL CLASS:				SAR: phenol – poly	
ECOTOX CONCERN	(H)	M	L	CONCERN CONCENTRATION	0.002
DATE 10/30/98				ASSESSOR:	

OPPT STRUCTURE ACTIVITY TEAM (SAT) MEETING DATE 11-3-98

	ATTENDEES	SIGNATURE
	CHEMISTRY	
✓	Paul Bickart	
	Diana Darling	
✓	Rich Engler	
	Greg Fritz	
	Fred Metz	
	Daniel Lin	
	ENVIRONMENTAL FATE	
	Bob Boethling	
	David Lynch	
✓	Gary Thom	
	HEALTH	
	Katherine Anitole	
✓	Michael Cimino	
	Leonard Keifer	
	David Lai	
✓	Jim Murphy	
✓	Deborah Norris	
	Ronald Ward	
✓	Yin Tak Woo	
	ENVIRONMENTAL EFFECTS	
✓	Gordon Cash	
	Vince Nabholz	
	Maggie Wilson	
	SAT CHAIRPERSON/OTHER	
	Rebecca Jones	
✓	Leonard Keifer	
	Vince Nabholz	
	Robert Morcock	